On the Temperature of Nonequilibrium Steady-State Systems

A. Baranyai
Department of Theoretical
Chemistry, Eötvös University
1518 Budapest 112
PO BOX 32, Hungary

We determined the operational temperatures of nonequilibrium molecular dynamics (NEMD) systems by our recently developed thermometer and compared these values to the dynamic temperatures [H. H. Rough, *Phys. Rev. Letter*, **78**, 772 (1997)] of the same systems. NEMD models use 'synthetic' thermostats, a numerical feedback procedure to remove the dissipative heat instantaneously. The impact of the feedback is to split up the dynamic temperature. The kinetic part is different from the configurational part because the energy is removed through the momentum sub-space of the system. In addition to this, these temperature values also depend on the direction. In the case of planar Couette flow, for dense liquids the operational temperature is close to the configurational temperature of the direction of the transverse momentum current. In the case of color conductivity, the operational temperature seems to be equal to the configurational temperature which, in contrast to the kinetic temperature of this model, is isotropic. We show that the experienced split of the dynamic temperature is an artifact of the instantaneous feedback of NEMD models. Since relaxation of a pre-set difference between the kinetic and the configurational temperature is an order of magnitude faster than relaxation of the heat flux vector, for models with realistic thermostats such a split cannot be observed. We argue that in real systems far from equilibrium the operational temperature and both terms of the dynamic temperature are identical and isotropic.